PERGAMON

Radiation Physics and Chemistry 58 (2000) 659–665

Radiation Physics and Chemistry

www.elsevier.com/locate/radphyschem

Positrons as probes of Si(100) surface with adsorbed hydrogen and oxygen

N.G. Fazleev[a, b,*], J.L. Fry[a], A.H. Weiss[a]

[a]*Department of Physics, Box 19059, The University of Texas at Arlington, Arlington, TX 76019-0059, USA*
[b]*Department of Physics, Kazan State University, Kazan 420008, Russia*

Abstract

Positron annihilation induced Auger spectra from the Si(100) surface exposed to hydrogen and oxygen are analyzed by performing calculations of positron surface states and annihilation characteristics of surface trapped positrons. Positron binding energies and work functions are also computed. It is found that the adsorption of hydrogen and oxygen on the Si(100) surface leads to a displacement of the positron surface state wave function away from the substrate Si atoms. As a result of this displacement, the overlap of the positron wave function with Si core electrons and, consequently, the annihilation probability of Si core electrons reduce, in agreement with experimental data.

1. Introduction

The adsorption of hydrogen and oxygen on a Si surface has attracted increased interest due to the applications of these processes in device technology. Hydrogen adsorption is used mostly to lower the surface energy of Si and thus stabilize the Si surface prior to molecular beam epitaxy. It is also used to produce an inactive Si surface for other device fabrication processes. However the difficulty of detecting hydrogen using standard surface spectroscopies leaves many open questions regarding the behavior of the absorbed hydrogen on a semiconductor surface. Oxygen adsorption is of interest due to its significance in Si device processing and in metal-oxide semiconductor device fabrication. Numerous studies of oxygen absorption have been directed towards better understanding of the formation of SiO_2 and a Si/SiO_2 interface. Nevertheless, the initial stages of oxidation of a semiconductor surface are still not well understood.

Recently the adsorption of hydrogen and oxygen on the Si(100) surface has become the subject of experimental studies using a novel surface characterization technique, positron-annihilation-induced Auger-electron spectroscopy (PAES) (Weiss, 1992; Kim et al., 1998). In PAES experiments, most of the low-energy positrons implanted into the sample under study diffuse back to the vacuum–solid interface and are trapped into a surface state. A certain fraction of surface-trapped positrons annihilate with neighboring core-level electrons, creating core-hole excitations and initiating Auger processes (almost exclusively in atoms in the topmost layer). Since PAES intensities are sensitive to the spatial distribution of the positron wave function at the surfaces of interest, the method has already been used to selectively obtain chemical information from the topmost atomic layer and to clarify the nature of the positron surface state (Weiss, 1993).

* Corresponding author. Fax: +1-817-272-3637.
E-mail address: fazleev@uta.edu (N.G. Fazleev).

0969-806X/00/$ - see front matter
PII: S0969-806X(00)00234-6